Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +) -5.60 ±1.55 (n=48)
logP (neutral X) 2.09 ±0.01 (n=48)

18B-27016 Points 1 to 20

M11_octanol concentration factor 0.990
Carbonate 0.0000 mM
Acidity error 0.67760 mM

18B-27016 Points 21 to 40

M11_octanol concentration factor 0.815
Carbonate 0.0822 mM
Acidity error 0.32858 mM

18B-27016 Points 41 to 62

M11_octanol concentration factor 0.703
Carbonate 0.1416 mM
Acidity error 0.69165 mM

Warnings and errors

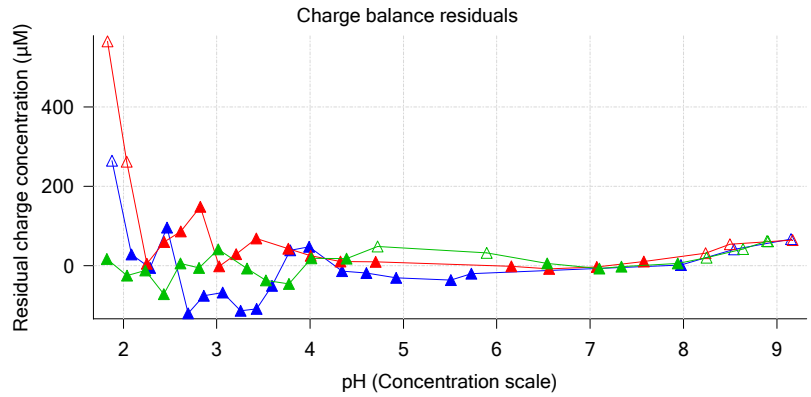
Errors None
Warnings One or more logP values out of range

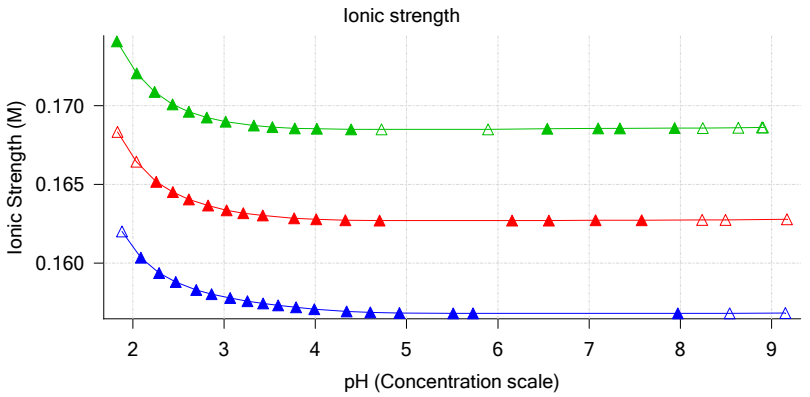
Sample logD and percent species

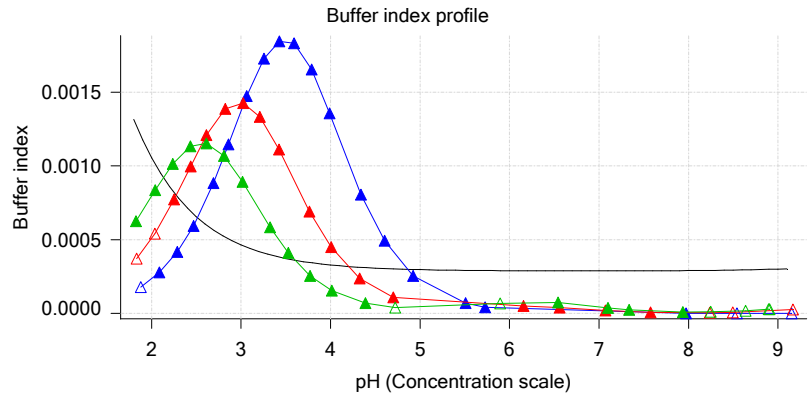
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.80	86.28 %	0.11 %	0.00 %	13.61 %	
1.200	-0.60	79.87 %	0.16 %	0.00 %	19.97 %	Stomach pH
2.000	0.19	38.61 %	0.50 %	0.00 %	60.90 %	
3.000	1.15	5.92 %	0.76 %	0.00 %	93.32 %	
4.000	1.84	0.62 %	0.81 %	0.00 %	98.57 %	
5.000	2.06	0.06 %	0.81 %	0.00 %	99.13 %	
6.000	2.08	0.01 %	0.81 %	0.00 %	99.18 %	
6.500	2.09	0.00 %	0.81 %	0.00 %	99.19 %	
7.000	2.09	0.00 %	0.81 %	0.00 %	99.19 %	
7.400	2.09	0.00 %	0.81 %	0.00 %	99.19 %	Blood pH
8.000	2.09	0.00 %	0.81 %	0.00 %	99.19 %	
9.000	2.09	0.00 %	0.81 %	0.00 %	99.19 %	
10.000	2.09	0.00 %	0.81 %	0.00 %	99.19 %	
11.000	2.09	0.00 %	0.81 %	0.00 %	99.19 %	
12.000	2.09	0.00 %	0.81 %	0.00 %	99.19 %	

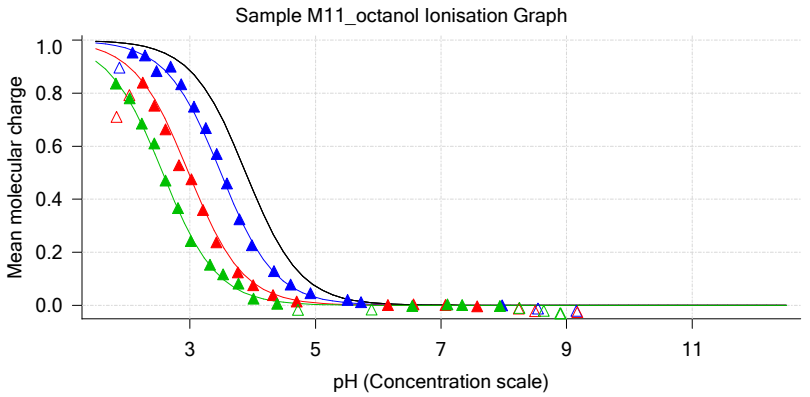
Sample name:	**M11_octanol**	Experiment start time:	**2/27/2018 10:54:30 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-27016**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**		

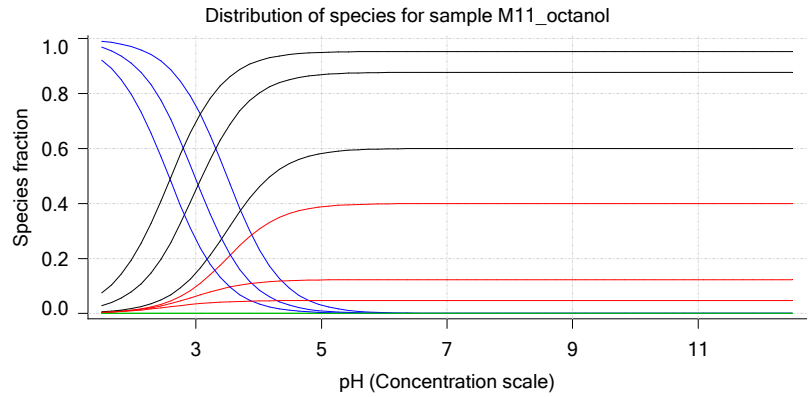
Graphs

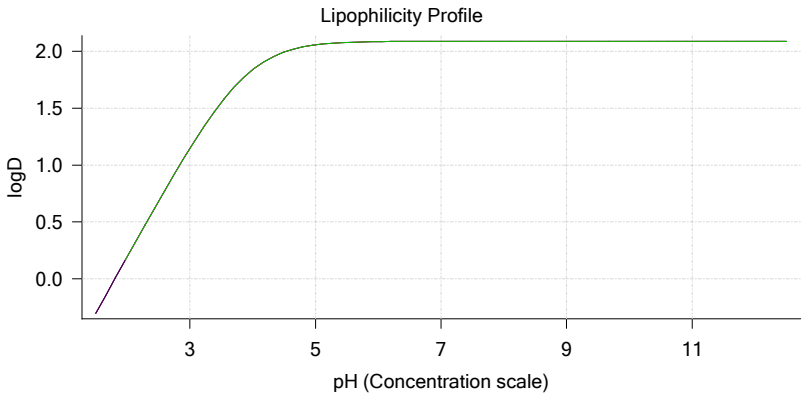


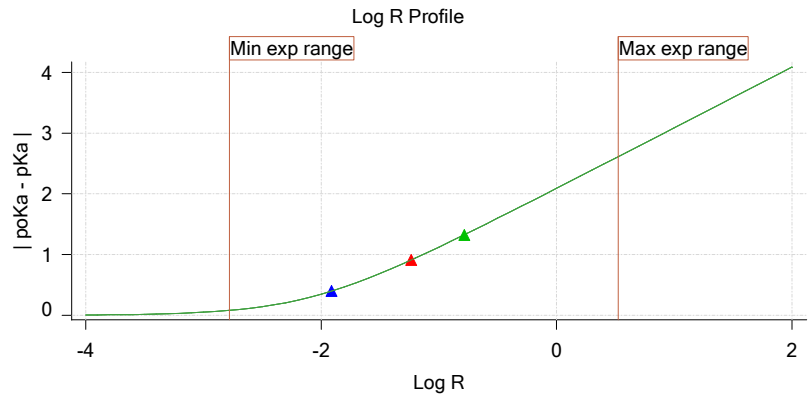


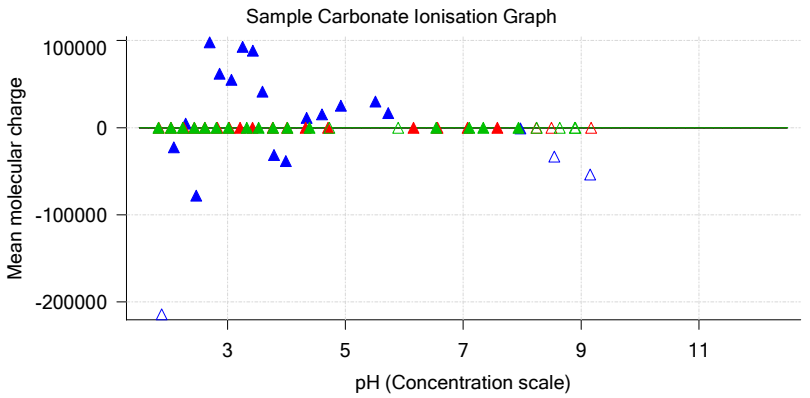








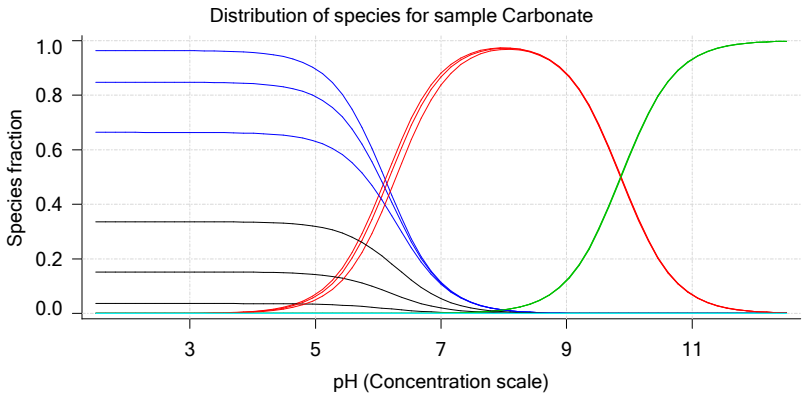




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M11_octanol**	Experiment start time:	**2/27/2018 10:54:30 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-27016**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18B-27016 Points 1 to 20

Overall results

RMSD	0.163
Average ionic strength	0.158 M
Average temperature	25.0°C
Partition ratio	0.0123 : 1
Analyte concentration range	3203.9 µM to 3307.2 µM
Total points considered	17 of 20

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r

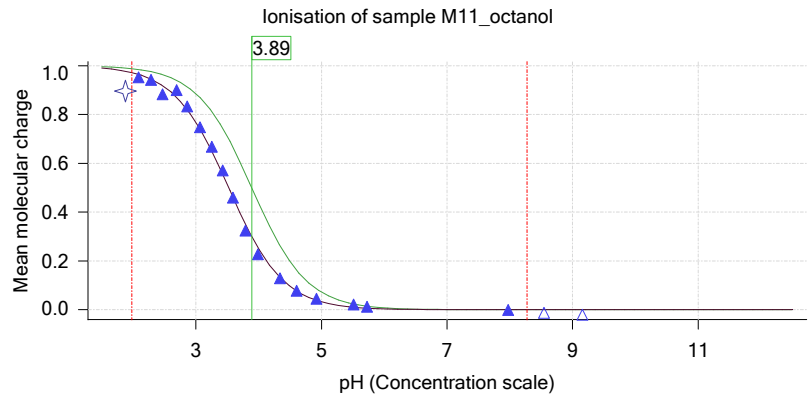
Titrants

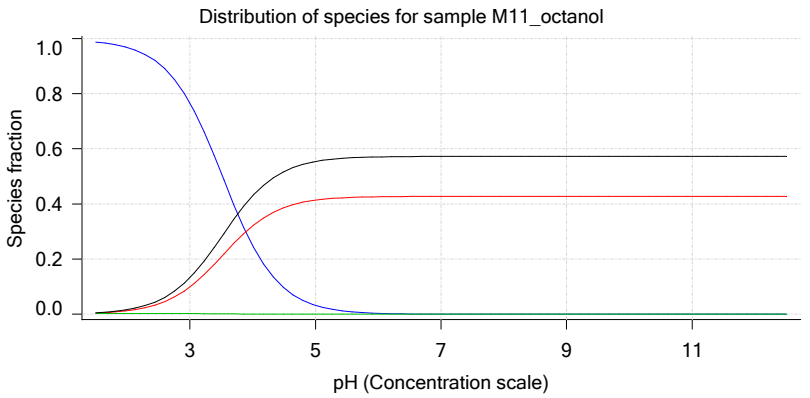
0.50 M HCl	0.993513	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/27/2018 10:54:30 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor	0.990
Base pKa 1	3.89
logP (XH +)	-0.58
logP (neutral X)	2.04

Sample graphs

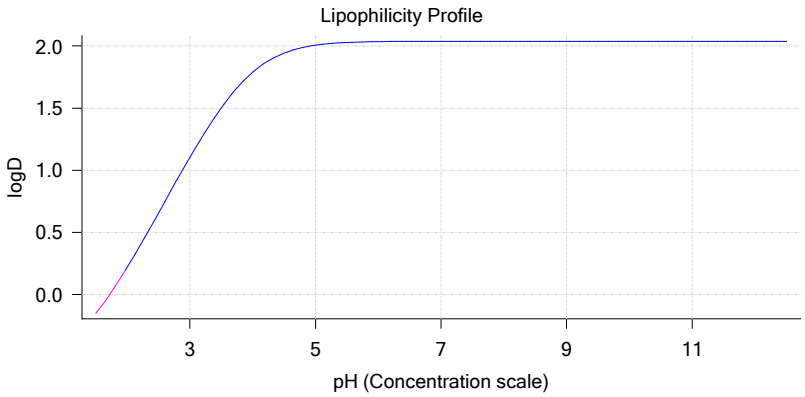




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



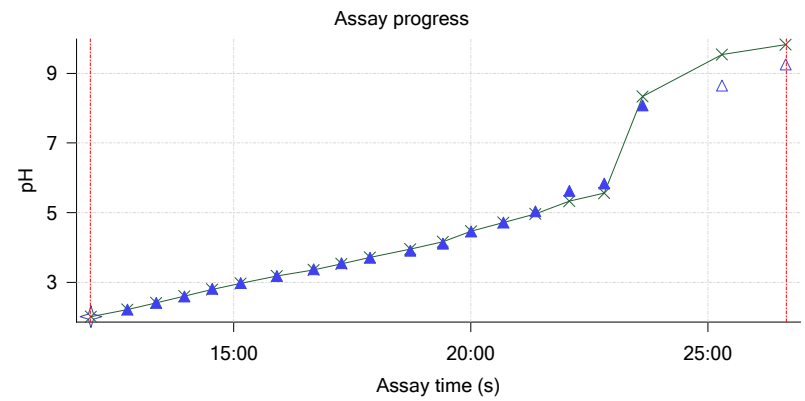
Sample logD and percent species

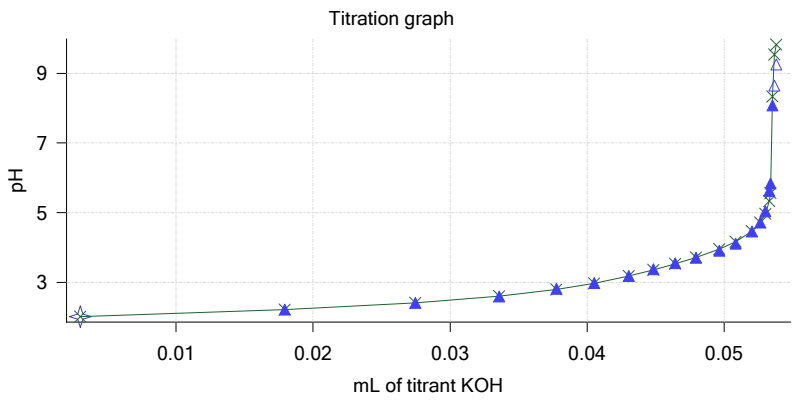
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.40	99.38 %	0.13 %	0.32 %	0.17 %	
1.200	-0.31	99.21 %	0.20 %	0.32 %	0.27 %	Stomach pH
2.000	0.22	96.77 %	1.25 %	0.31 %	1.67 %	
3.000	1.10	76.66 %	9.88 %	0.25 %	13.22 %	
4.000	1.79	24.90 %	32.08 %	0.08 %	42.94 %	
5.000	2.01	3.21 %	41.38 %	0.01 %	55.40 %	
6.000	2.03	0.33 %	42.61 %	0.00 %	57.05 %	
6.500	2.04	0.10 %	42.71 %	0.00 %	57.18 %	
7.000	2.04	0.03 %	42.74 %	0.00 %	57.22 %	
7.400	2.04	0.01 %	42.75 %	0.00 %	57.24 %	Blood pH
8.000	2.04	0.00 %	42.76 %	0.00 %	57.24 %	
9.000	2.04	0.00 %	42.76 %	0.00 %	57.24 %	
10.000	2.04	0.00 %	42.76 %	0.00 %	57.24 %	
11.000	2.04	0.00 %	42.76 %	0.00 %	57.24 %	
12.000	2.04	0.00 %	42.76 %	0.00 %	57.24 %	

Carbonate and acidity

Carbonate 0.000 mM
Acidity error 0.678 mM

Other graphs

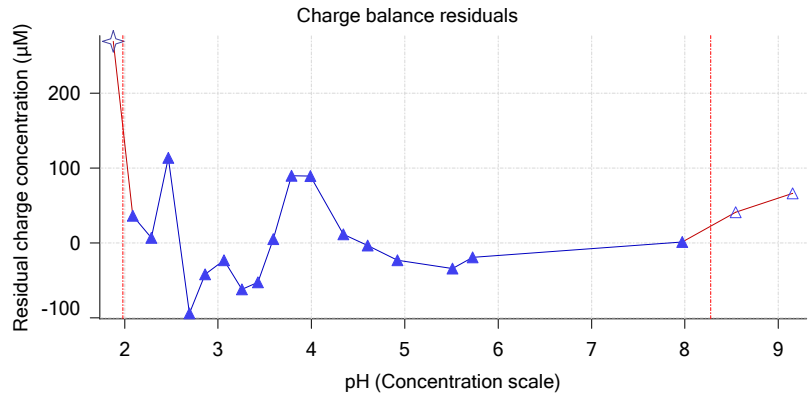


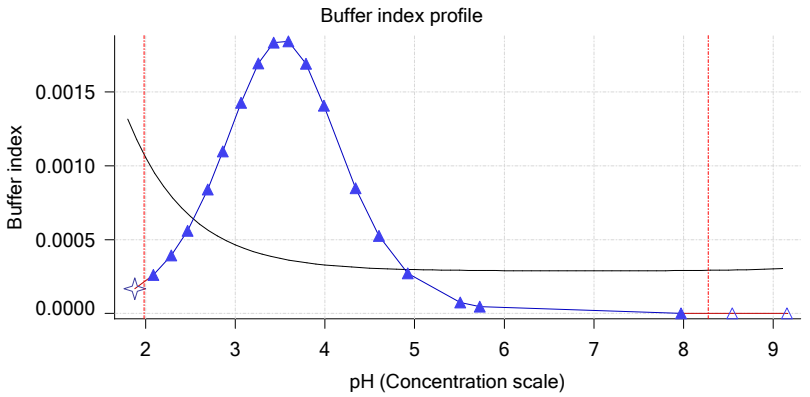


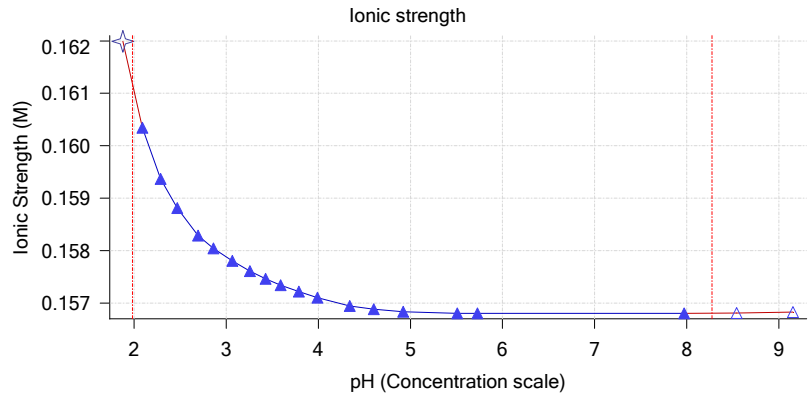
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

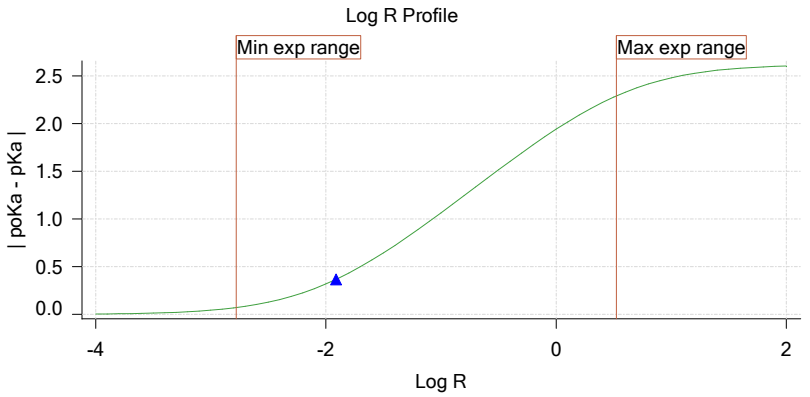
Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

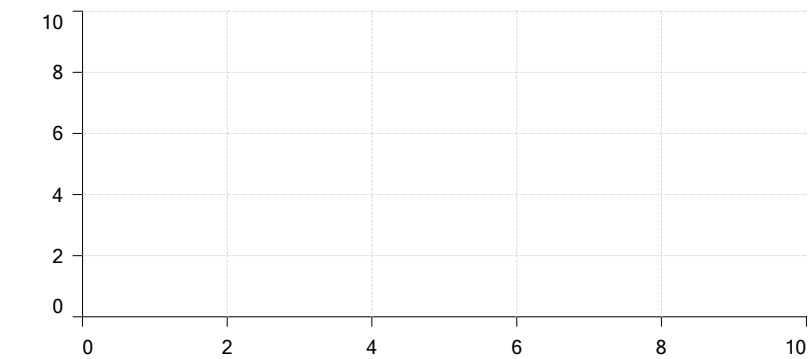
Other graphs (continued)

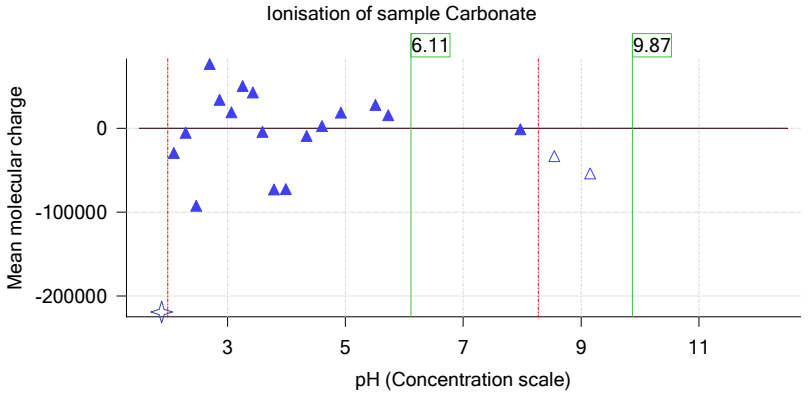












Sample name:	**M11_octanol**	Experiment start time:	**2/27/2018 10:54:30 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-27016**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18B-27016 Points 21 to 40

Overall results

RMSD	0.275
Average ionic strength	0.163 M
Average temperature	25.0°C
Partition ratio	0.0582 : 1
Analyte concentration range	2864.7 µM to 2955.2 µM
Total points considered	15 of 20

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r

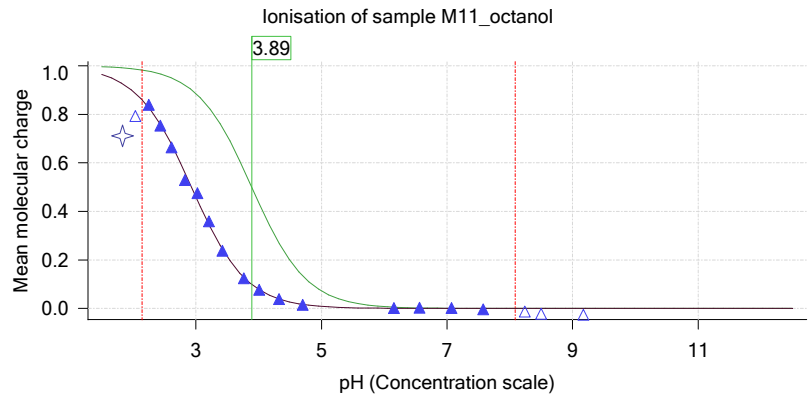
Titrants

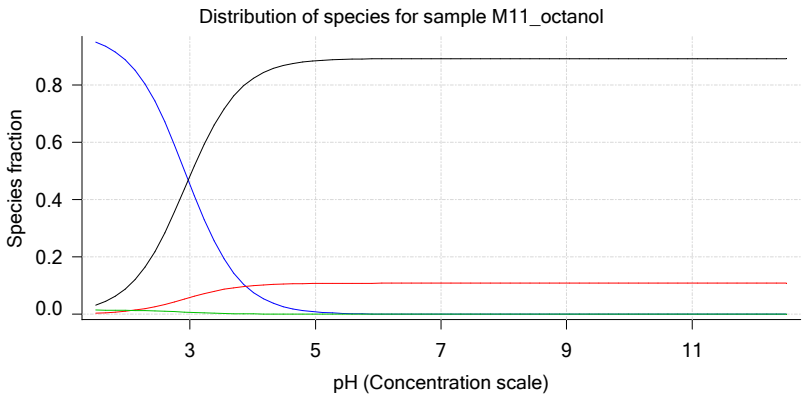
0.50 M HCl	0.993513	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/27/2018 10:54:30 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor	0.815
Base pKa 1	3.89
logP (XH +)	-0.58
logP (neutral X)	2.15

Sample graphs

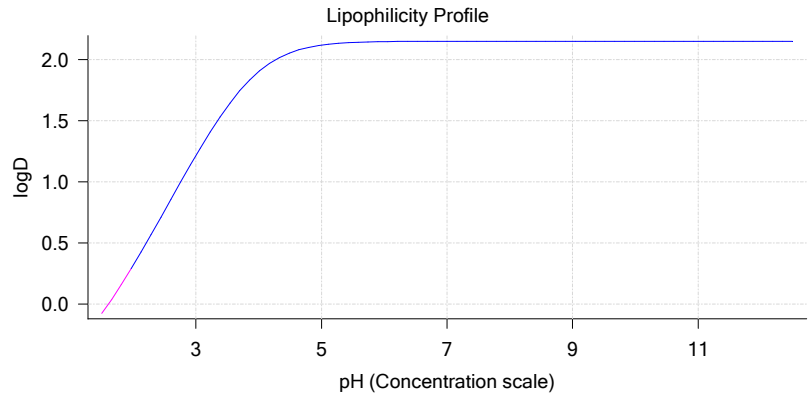




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



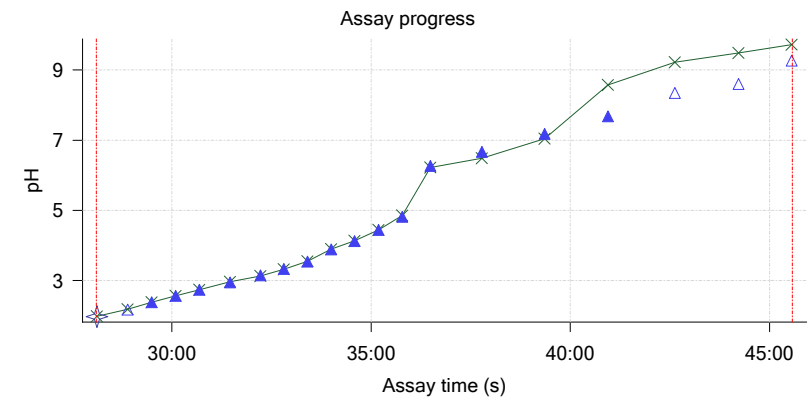
Sample logD and percent species

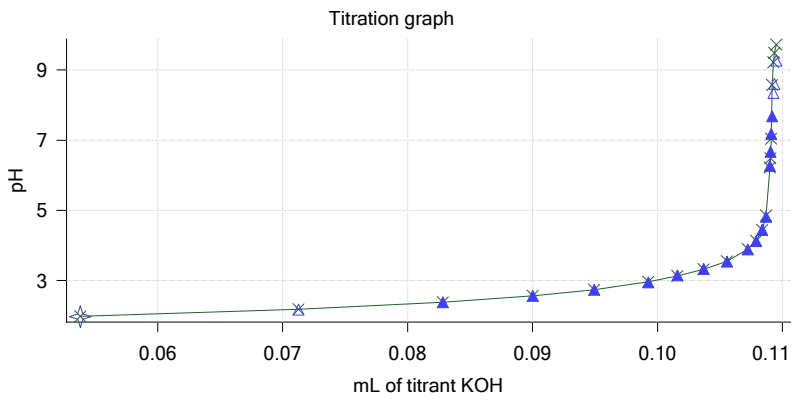
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.35	97.35 %	0.13 %	1.49 %	1.03 %	
1.200	-0.26	96.70 %	0.20 %	1.48 %	1.63 %	Stomach pH
2.000	0.31	88.17 %	1.14 %	1.35 %	9.35 %	
3.000	1.21	45.36 %	5.84 %	0.69 %	48.10 %	
4.000	1.90	7.75 %	9.98 %	0.12 %	82.15 %	
5.000	2.12	0.83 %	10.74 %	0.01 %	88.41 %	
6.000	2.15	0.08 %	10.82 %	0.00 %	89.09 %	
6.500	2.15	0.03 %	10.83 %	0.00 %	89.14 %	
7.000	2.15	0.01 %	10.83 %	0.00 %	89.16 %	
7.400	2.15	0.00 %	10.83 %	0.00 %	89.16 %	Blood pH
8.000	2.15	0.00 %	10.83 %	0.00 %	89.17 %	
9.000	2.15	0.00 %	10.83 %	0.00 %	89.17 %	
10.000	2.15	0.00 %	10.83 %	0.00 %	89.17 %	
11.000	2.15	0.00 %	10.83 %	0.00 %	89.17 %	
12.000	2.15	0.00 %	10.83 %	0.00 %	89.17 %	

Carbonate and acidity

Carbonate 0.082 mM
Acidity error 0.329 mM

Other graphs

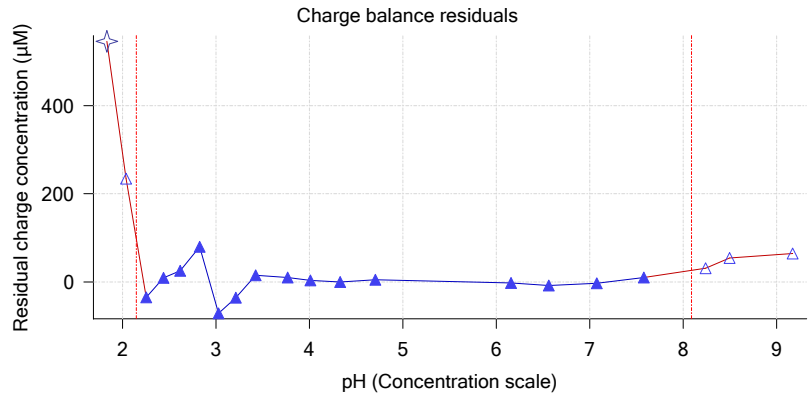


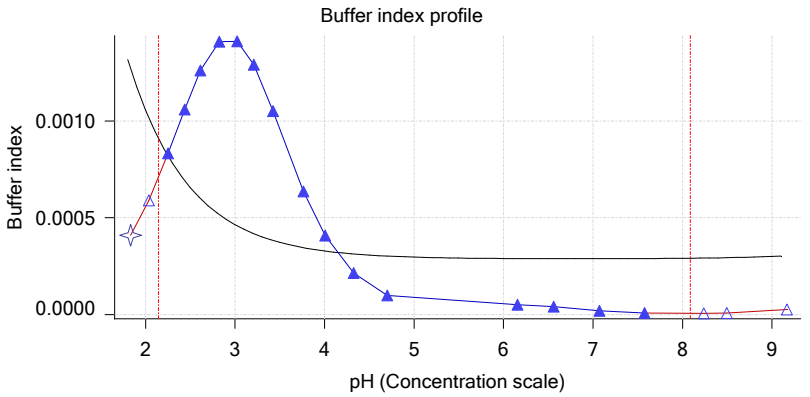


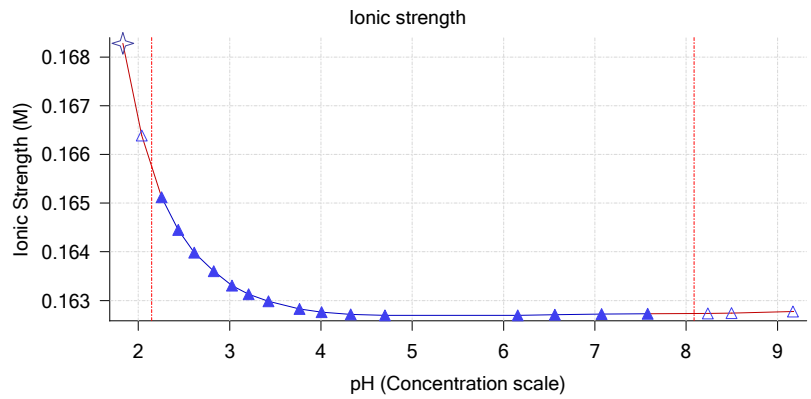
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

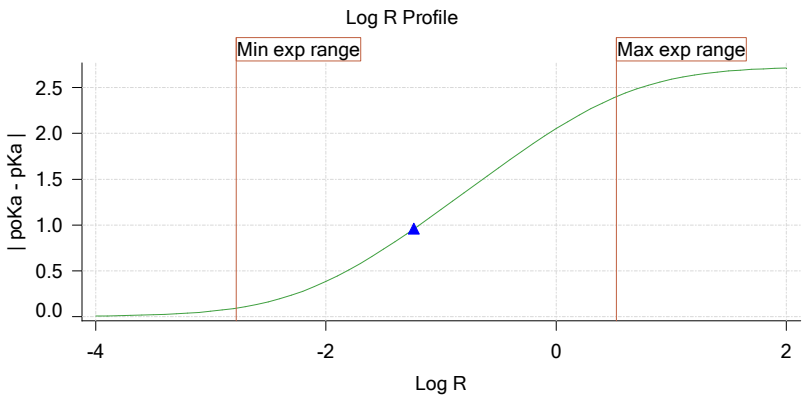
Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

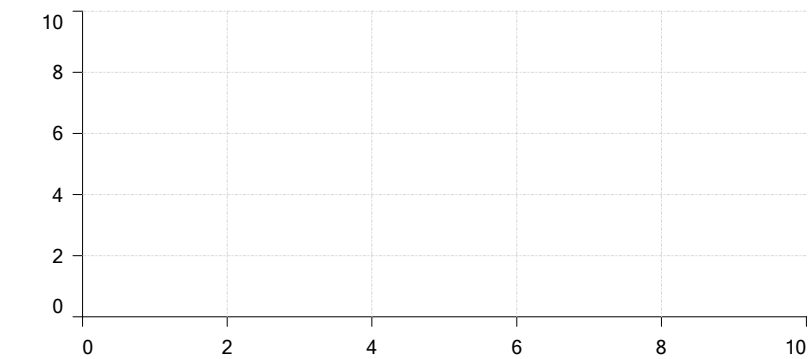
Other graphs (continued)

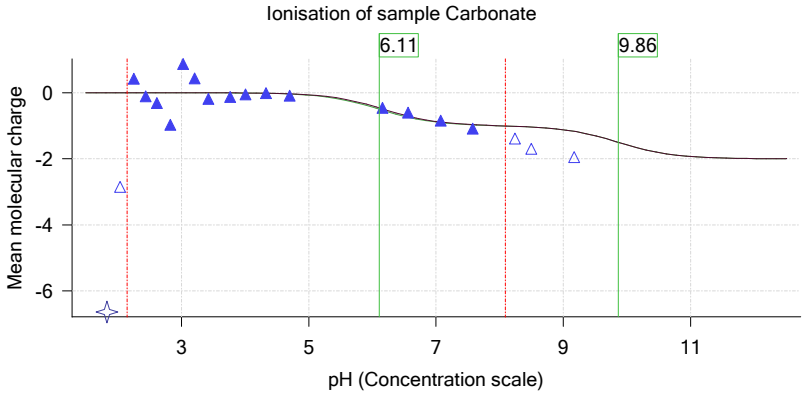












Sample name:	**M11_octanol**	Experiment start time:	**2/27/2018 10:54:30 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-27016**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18B-27016 Points 41 to 62

Overall results

RMSD	0.122
Average ionic strength	0.169 M
Average temperature	25.0°C
Partition ratio	0.1640 : 1
Analyte concentration range	2436.6 µM to 2507.4 µM
Total points considered	16 of 22

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r

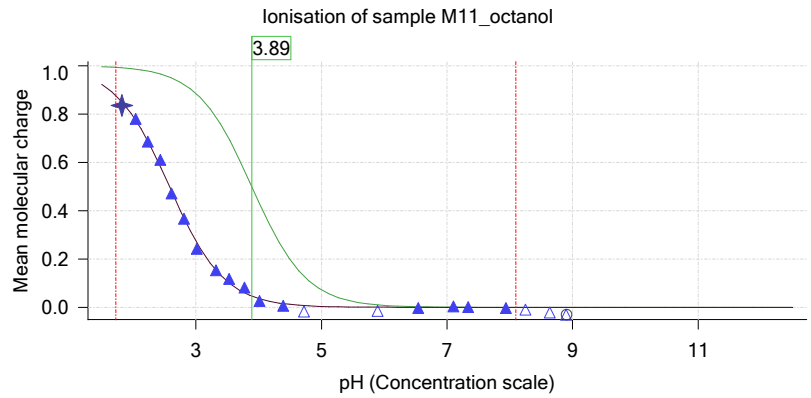
Titrants

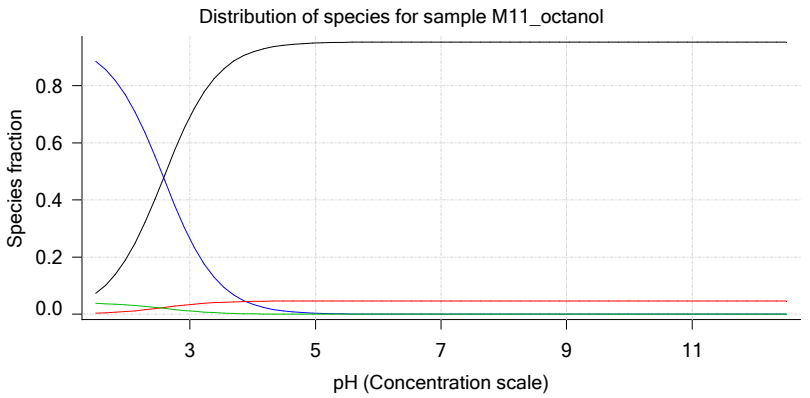
0.50 M HCl	0.993513	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/27/2018 10:54:30 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor	0.703
Base pKa 1	3.89
logP (XH +)	-0.58
logP (neutral X)	2.09

Sample graphs

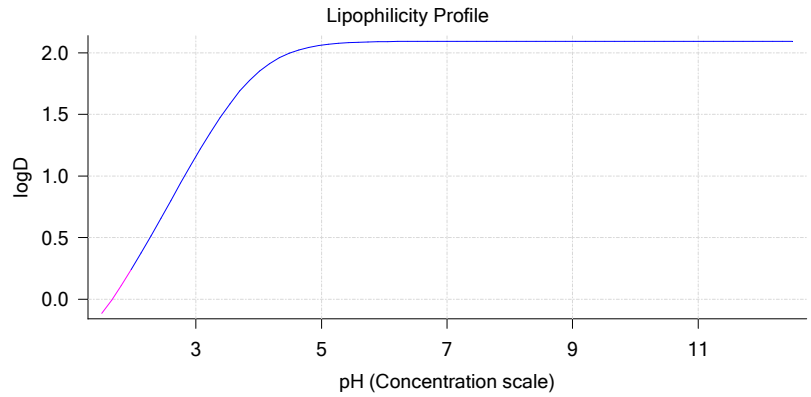




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



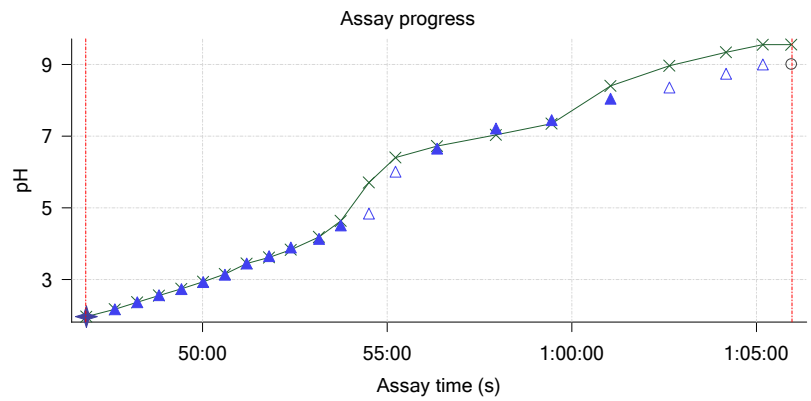
Sample logD and percent species

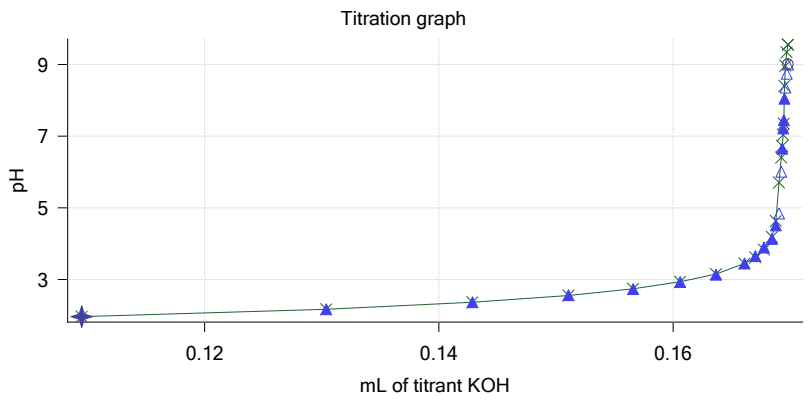
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.37	93.40 %	0.12 %	4.03 %	2.45 %	
1.200	-0.29	92.02 %	0.19 %	3.97 %	3.82 %	Stomach pH
2.000	0.26	75.86 %	0.98 %	3.27 %	19.89 %	
3.000	1.16	26.36 %	3.40 %	1.14 %	69.10 %	
4.000	1.84	3.50 %	4.51 %	0.15 %	91.83 %	
5.000	2.06	0.36 %	4.67 %	0.02 %	94.96 %	
6.000	2.09	0.04 %	4.68 %	0.00 %	95.28 %	
6.500	2.09	0.01 %	4.68 %	0.00 %	95.30 %	
7.000	2.09	0.00 %	4.68 %	0.00 %	95.31 %	
7.400	2.09	0.00 %	4.68 %	0.00 %	95.31 %	Blood pH
8.000	2.09	0.00 %	4.68 %	0.00 %	95.32 %	
9.000	2.09	0.00 %	4.68 %	0.00 %	95.32 %	
10.000	2.09	0.00 %	4.68 %	0.00 %	95.32 %	
11.000	2.09	0.00 %	4.68 %	0.00 %	95.32 %	
12.000	2.09	0.00 %	4.68 %	0.00 %	95.32 %	

Carbonate and acidity

Carbonate 0.142 mM
Acidity error 0.692 mM

Other graphs

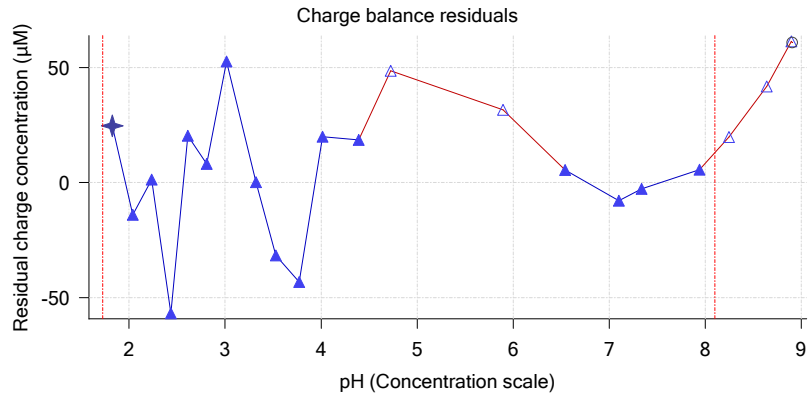


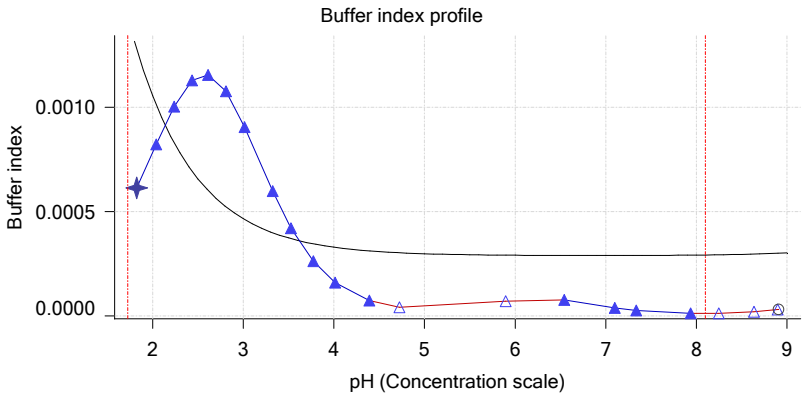


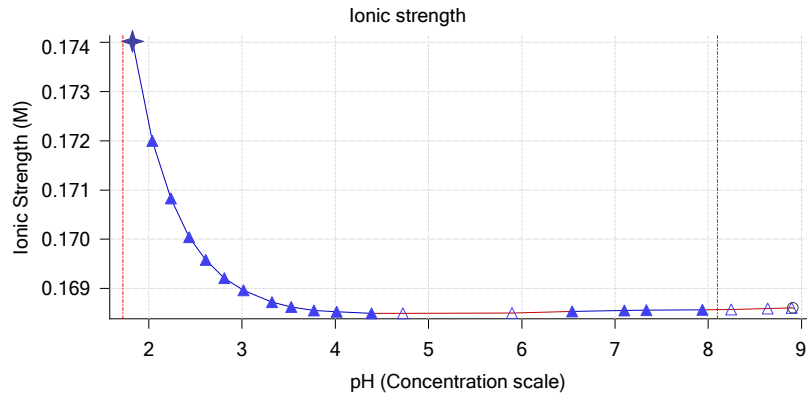
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

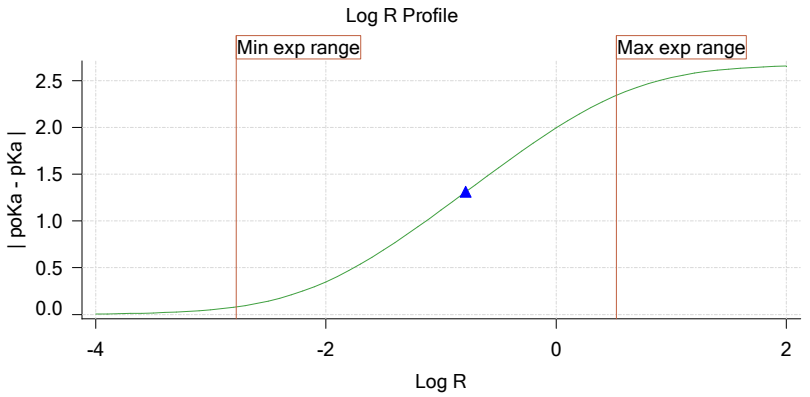
Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

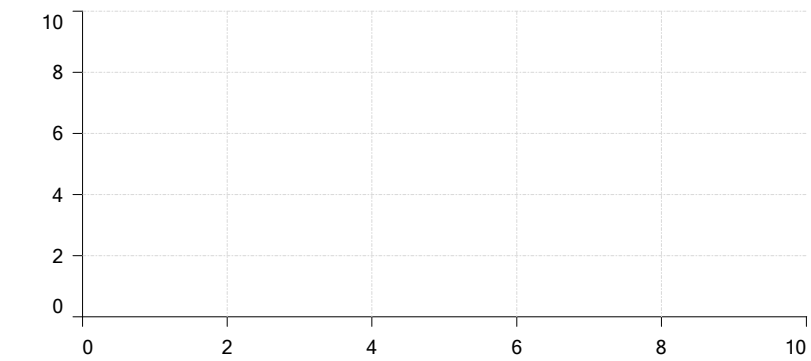
Other graphs (continued)

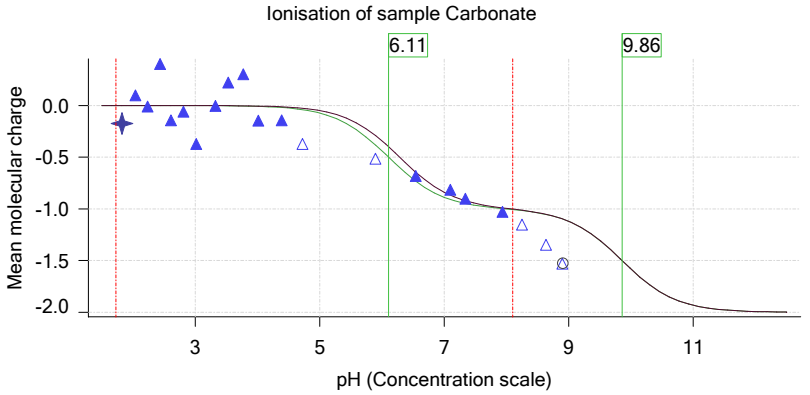












Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M11_octanol	2/27/2018 4:54:30 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001100 g	2/27/2018 6:40:56 PM	User entered value
Formula weight	211.22 g/mol	2/27/2018 4:54:30 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	211.22	2/27/2018 4:54:30 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:54:30 PM	User entered value
Sample is a	Base	2/27/2018 4:54:30 PM	User entered value
pKa 1	3.89	2/27/2018 4:54:30 PM	User entered value
logp (XH +)	-0.58	2/27/2018 4:54:54 PM	User entered value
logP (neutral X)	1.24	2/27/2018 4:54:49 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
8:60.0	Initial pH = 6.35									
11:59.5	Data point 1	1.50000 mL	0.05167 mL	0.00301 mL	0.01999 mL	2.012	-0.01321	0.59861	0.00084	10.0 s
12:45.7	Data point 2	1.50000 mL	0.05167 mL	0.01794 mL	0.01999 mL	2.217	-0.01201	0.89280	0.00063	10.5 s
13:21.8	Data point 3	1.50000 mL	0.05167 mL	0.02747 mL	0.01999 mL	2.415	-0.00642	0.73636	0.00037	10.0 s
13:57.4	Data point 4	1.50000 mL	0.05167 mL	0.03358 mL	0.01999 mL	2.593	-0.00697	0.59547	0.00045	10.0 s
14:32.9	Data point 5	1.50000 mL	0.05167 mL	0.03777 mL	0.01999 mL	2.816	-0.00524	0.75021	0.00030	10.5 s
15:08.9	Data point 6	1.50000 mL	0.05167 mL	0.04052 mL	0.01999 mL	2.984	-0.01107	0.79804	0.00061	10.0 s
15:54.8	Data point 7	1.50000 mL	0.05167 mL	0.04304 mL	0.01999 mL	3.186	-0.00468	0.88101	0.00025	10.5 s
16:41.1	Data point 8	1.50000 mL	0.05167 mL	0.04485 mL	0.01999 mL	3.377	-0.00932	0.44692	0.00069	10.0 s
17:16.6	Data point 9	1.50000 mL	0.05167 mL	0.04643 mL	0.01999 mL	3.547	-0.00399	0.79959	0.00022	10.5 s
17:52.6	Data point 10	1.50000 mL	0.05167 mL	0.04795 mL	0.01999 mL	3.710	-0.00939	0.88441	0.00049	10.0 s
18:43.6	Data point 11	1.50000 mL	0.05167 mL	0.04965 mL	0.01999 mL	3.906	0.00461	0.20532	0.00050	10.5 s
19:24.7	Data point 12	1.50000 mL	0.05167 mL	0.05085 mL	0.01999 mL	4.108	-0.01572	0.89585	0.00082	10.0 s
20:00.3	Data point 13	1.50000 mL	0.05167 mL	0.05205 mL	0.01999 mL	4.458	-0.01283	0.78922	0.00071	10.5 s
20:41.3	Data point 14	1.50000 mL	0.05167 mL	0.05263 mL	0.01999 mL	4.719	-0.01182	0.87243	0.00063	10.0 s
21:21.9	Data point 15	1.50000 mL	0.05167 mL	0.05301 mL	0.01999 mL	5.038	-0.01739	0.94532	0.00088	12.5 s
22:05.0	Data point 16	1.50000 mL	0.05167 mL	0.05329 mL	0.01999 mL	5.624	-0.01784	0.80310	0.00098	18.5 s
22:48.9	Data point 17	1.50000 mL	0.05167 mL	0.05339 mL	0.01999 mL	5.840	-0.01669	0.76560	0.00094	18.0 s
23:37.4	Data point 18	1.50000 mL	0.05167 mL	0.05353 mL	0.01999 mL	8.078	-0.05197	0.99587	0.00257	Timed out at 59.5 s
25:18.2	Data point 19	1.50000 mL	0.05167 mL	0.05367 mL	0.01999 mL	8.647	-0.01738	0.86596	0.00092	44.5 s
26:38.3	Data point 20	1.50000 mL	0.05167 mL	0.05381 mL	0.01999 mL	9.256	-0.01881	0.92735	0.00096	29.0 s
28:07.4	Data point 21	1.50000 mL	0.10842 mL	0.05381 mL	0.10000 mL	1.967	-0.00520	0.28864	0.00048	10.0 s
28:53.7	Data point 22	1.50000 mL	0.10842 mL	0.07126 mL	0.10000 mL	2.168	-0.01928	0.91140	0.00100	10.5 s
29:29.9	Data point 23	1.50000 mL	0.10842 mL	0.08283 mL	0.10000 mL	2.381	0.00042	0.05097	0.00009	10.5 s
30:06.0	Data point 24	1.50000 mL	0.10842 mL	0.09000 mL	0.10000 mL	2.562	-0.00366	0.61217	0.00023	10.0 s
30:41.6	Data point 25	1.50000 mL	0.10842 mL	0.09492 mL	0.10000 mL	2.738	-0.01006	0.31818	0.00088	10.0 s
31:27.5	Data point 26	1.50000 mL	0.10842 mL	0.09925 mL	0.10000 mL	2.947	-0.00503	0.77202	0.00028	10.0 s
32:13.3	Data point 27	1.50000 mL	0.10842 mL	0.10160 mL	0.10000 mL	3.147	-0.00762	0.61374	0.00048	10.0 s
32:48.8	Data point 28	1.50000 mL	0.10842 mL	0.10369 mL	0.10000 mL	3.331	-0.01378	0.87687	0.00073	10.0 s
33:24.3	Data point 29	1.50000 mL	0.10842 mL	0.10555 mL	0.10000 mL	3.544	-0.00880	0.29642	0.00080	10.0 s
33:59.7	Data point 30	1.50000 mL	0.10842 mL	0.10722 mL	0.10000 mL	3.884	-0.00929	0.26981	0.00088	10.0 s
34:35.2	Data point 31	1.50000 mL	0.10842 mL	0.10788 mL	0.10000 mL	4.125	-0.00452	0.80460	0.00025	10.5 s
35:11.1	Data point 32	1.50000 mL	0.10842 mL	0.10837 mL	0.10000 mL	4.444	-0.01177	0.87839	0.00062	10.5 s
35:46.9	Data point 33	1.50000 mL	0.10842 mL	0.10868 mL	0.10000 mL	4.818	-0.01577	0.78042	0.00088	12.0 s
36:29.4	Data point 34	1.50000 mL	0.10842 mL	0.10898 mL	0.10000 mL	6.267	-0.01927	0.97409	0.00096	52.0 s
37:46.9	Data point 35	1.50000 mL	0.10842 mL	0.10903 mL	0.10000 mL	6.671	-0.01898	0.96189	0.00096	58.5 s
39:21.1	Data point 36	1.50000 mL	0.10842 mL	0.10910 mL	0.10000 mL	7.182	-0.05514	0.98470	0.00274	Timed out at 59.5 s
40:56.7	Data point 37	1.50000 mL	0.10842 mL	0.10917 mL	0.10000 mL	7.684	-0.05926	0.99557	0.00293	Timed out at 59.5 s

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
42:37.4	Data point 38	1.50000 mL	0.10842 mL	0.10927 mL	0.10000 mL	8.344	-0.02444	0.97413	0.00122	Timed out at 59.5 s
44:13.0	Data point 39	1.50000 mL	0.10842 mL	0.10936 mL	0.10000 mL	8.601	-0.01930	0.94203	0.00098	44.5 s
45:33.1	Data point 40	1.50000 mL	0.10842 mL	0.10950 mL	0.10000 mL	9.271	-0.01442	0.69862	0.00085	15.0 s
46:50.9	Data point 41	1.50000 mL	0.16747 mL	0.10950 mL	0.30000 mL	1.960	-0.00611	0.71181	0.00036	10.0 s
47:37.4	Data point 42	1.50000 mL	0.16747 mL	0.13039 mL	0.30000 mL	2.171	-0.01056	0.60425	0.00067	10.5 s
48:13.6	Data point 43	1.50000 mL	0.16747 mL	0.14287 mL	0.30000 mL	2.364	-0.00724	0.54028	0.00049	10.0 s
48:49.2	Data point 44	1.50000 mL	0.16747 mL	0.15106 mL	0.30000 mL	2.559	-0.00372	0.68600	0.00022	10.5 s
49:25.4	Data point 45	1.50000 mL	0.16747 mL	0.15656 mL	0.30000 mL	2.736	-0.00396	0.44516	0.00029	10.0 s
50:00.9	Data point 46	1.50000 mL	0.16747 mL	0.16058 mL	0.30000 mL	2.932	-0.00663	0.33641	0.00056	10.0 s
50:36.4	Data point 47	1.50000 mL	0.16747 mL	0.16364 mL	0.30000 mL	3.137	-0.01016	0.30029	0.00092	10.0 s
51:11.9	Data point 48	1.50000 mL	0.16747 mL	0.16609 mL	0.30000 mL	3.444	-0.00956	0.44143	0.00071	10.5 s
51:47.9	Data point 49	1.50000 mL	0.16747 mL	0.16700 mL	0.30000 mL	3.647	-0.00982	0.27260	0.00093	10.0 s
52:23.4	Data point 50	1.50000 mL	0.16747 mL	0.16773 mL	0.30000 mL	3.891	-0.00230	0.16102	0.00028	10.0 s
53:09.1	Data point 51	1.50000 mL	0.16747 mL	0.16842 mL	0.30000 mL	4.133	-0.00752	0.36746	0.00061	10.0 s
53:44.5	Data point 52	1.50000 mL	0.16747 mL	0.16877 mL	0.30000 mL	4.507	-0.01597	0.71656	0.00093	10.0 s
54:30.2	Data point 53	1.50000 mL	0.16747 mL	0.16903 mL	0.30000 mL	4.840	-0.00857	0.27004	0.00082	12.5 s
55:13.3	Data point 54	1.50000 mL	0.16747 mL	0.16921 mL	0.30000 mL	6.006	-0.01875	0.96219	0.00094	37.5 s
56:21.2	Data point 55	1.50000 mL	0.16747 mL	0.16931 mL	0.30000 mL	6.652	-0.05803	0.99479	0.00287	Timed out at 59.5 s
57:56.8	Data point 56	1.50000 mL	0.16747 mL	0.16938 mL	0.30000 mL	7.209	-0.06064	0.98448	0.00302	Timed out at 59.5 s
59:27.4	Data point 57	1.50000 mL	0.16747 mL	0.16943 mL	0.30000 mL	7.445	-0.06310	0.99629	0.00312	Timed out at 59.5 s
1:01:03.0	Data point 58	1.50000 mL	0.16747 mL	0.16950 mL	0.30000 mL	8.044	-0.04412	0.95409	0.00223	Timed out at 59.5 s
1:02:38.8	Data point 59	1.50000 mL	0.16747 mL	0.16957 mL	0.30000 mL	8.352	-0.01985	0.97791	0.00099	51.0 s
1:04:10.8	Data point 60	1.50000 mL	0.16747 mL	0.16969 mL	0.30000 mL	8.741	-0.01671	0.79899	0.00092	24.0 s
1:05:10.6	Data point 61	1.50000 mL	0.16747 mL	0.16980 mL	0.30000 mL	8.999	-0.01827	0.88409	0.00096	26.0 s
1:05:56.8	Data point 62	1.50000 mL	0.16747 mL	0.16980 mL	0.30000 mL	9.010	-0.01788	0.90579	0.00093	19.0 s
1:06:25.0	Assay volumes	1.50000 mL	0.16747 mL	0.16980 mL	0.30000 mL					

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.080 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**
Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	2/27/2018 10:54:30 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	2/27/2018 10:54:30 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	1/31/2018 12:26:26 PM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+2.59 mV		2/27/2018 10:54:58 PM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/27/2018 9:49:58 AM
Wash 2	0.5% Trition X-100 in H20		2/27/2018 9:50:01 AM
Buffer position 1	pH7 Wash		2/27/2018 9:50:04 AM
Buffer position 2	pH 7		2/27/2018 9:50:06 AM
Storage position			2/27/2018 9:55:12 AM
Wash water	9.2e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	6.2e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	110:52:56		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:08] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[8:53] Titrator arm moved to Titration position
[8:53] Argon flow rate set to 100
[8:53] Stirrer speed set to 10
[8:58] Automatically add 0.02000 mL of Octanol
[8:59] Dispensed 0.019991 mL of Octanol
[9:00] Initial pH = 6.35
[9:00] Iterative adjust 6.35 -> 2.00
[9:00] pH 6.35 -> 2.00
[9:02] Air gap released for Acid (0.5 M HCl)
[9:02] Dispensed 0.051670 mL of Acid (0.5 M HCl)
[9:08] Holding pH 2.00
[11:08] Stirrer speed set to 0
[11:08] Stirrer speed set to 50
[11:08] Iterative adjust 1.97 -> 2.00
[11:08] pH 1.97 -> 2.00
[11:08] Air gap released for Base (0.5 M KOH)
[11:09] Dispensed 0.003010 mL of Base (0.5 M KOH)
[11:59] Stirrer speed set to 0
[12:10] Datapoint id 1 collected
[12:10] Stirrer speed set to 50
[12:15] pH 2.02 -> 2.22
[12:15] Using cautious pH adjust
[12:15] Dispensed 0.007573 mL of Base (0.5 M KOH)
[12:20] Stepping pH = 2.11
[12:20] Dispensed 0.005950 mL of Base (0.5 M KOH)
[12:25] Stepping pH = 2.20
[12:25] Dispensed 0.001411 mL of Base (0.5 M KOH)
[12:31] Stepping pH = 2.22
[12:46] Stirrer speed set to 0
[12:56] Datapoint id 2 collected
[12:56] Charge balance equation is out by 1.4%
[12:56] Stirrer speed set to 50

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:01] pH 2.22 -> 2.42
[13:01] Using charge balance adjust
[13:02] Dispensed 0.009525 mL of Base (0.5 M KOH)
[13:22] Stirrer speed set to 0
[13:32] Datapoint id 3 collected
[13:32] Charge balance equation is out by -4.9%
[13:32] Stirrer speed set to 50
[13:37] pH 2.42 -> 2.62
[13:37] Using charge balance adjust
[13:37] Dispensed 0.006115 mL of Base (0.5 M KOH)
[13:57] Stirrer speed set to 0
[14:07] Datapoint id 4 collected
[14:07] Charge balance equation is out by -14.8%
[14:07] Stirrer speed set to 50
[14:12] pH 2.60 -> 2.80
[14:12] Using charge balance adjust
[14:13] Dispensed 0.004186 mL of Base (0.5 M KOH)
[14:33] Stirrer speed set to 0
[14:43] Datapoint id 5 collected
[14:43] Charge balance equation is out by 7.6%
[14:43] Stirrer speed set to 50
[14:48] pH 2.82 -> 3.02
[14:48] Using charge balance adjust
[14:49] Dispensed 0.002752 mL of Base (0.5 M KOH)
[15:09] Stirrer speed set to 0
[15:19] Datapoint id 6 collected
[15:19] Charge balance equation is out by -19.4%
[15:19] Stirrer speed set to 50
[15:24] pH 2.99 -> 3.19
[15:24] Using cautious pH adjust
[15:24] Dispensed 0.001058 mL of Base (0.5 M KOH)
[15:29] Stepping pH = 3.06
[15:29] Dispensed 0.001152 mL of Base (0.5 M KOH)
[15:34] Stepping pH = 3.16
[15:35] Dispensed 0.000306 mL of Base (0.5 M KOH)
[15:40] Stepping pH = 3.19
[15:55] Stirrer speed set to 0
[16:05] Datapoint id 7 collected
[16:05] Charge balance equation is out by -18.8%
[16:05] Stirrer speed set to 50
[16:10] pH 3.19 -> 3.39
[16:10] Using cautious pH adjust
[16:10] Dispensed 0.000870 mL of Base (0.5 M KOH)
[16:16] Stepping pH = 3.28
[16:16] Dispensed 0.000706 mL of Base (0.5 M KOH)
[16:21] Stepping pH = 3.36
[16:21] Dispensed 0.000235 mL of Base (0.5 M KOH)
[16:26] Stepping pH = 3.38
[16:41] Stirrer speed set to 0
[16:51] Datapoint id 8 collected
[16:51] Charge balance equation is out by -2.8%
[16:51] Stirrer speed set to 50
[16:56] pH 3.38 -> 3.58
[16:56] Using charge balance adjust
[16:56] Dispensed 0.001576 mL of Base (0.5 M KOH)
[17:17] Stirrer speed set to 0
[17:27] Datapoint id 9 collected
[17:27] Charge balance equation is out by -14.9%
[17:27] Stirrer speed set to 50

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:32] pH 3.55 -> 3.75
[17:32] Using charge balance adjust
[17:32] Dispensed 0.001529 mL of Base (0.5 M KOH)
[17:53] Stirrer speed set to 0
[18:03] Datapoint id 10 collected
[18:03] Charge balance equation is out by -21.5%
[18:03] Stirrer speed set to 50
[18:08] pH 3.71 -> 3.91
[18:08] Using cautious pH adjust
[18:08] Dispensed 0.000729 mL of Base (0.5 M KOH)
[18:13] Stepping pH = 3.79
[18:13] Dispensed 0.000729 mL of Base (0.5 M KOH)
[18:18] Stepping pH = 3.89
[18:18] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:23] Stepping pH = 3.90
[18:23] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:28] Stepping pH = 3.91
[18:44] Stirrer speed set to 0
[18:54] Datapoint id 11 collected
[18:54] Charge balance equation is out by -16.0%
[18:54] Stirrer speed set to 50
[18:59] pH 3.91 -> 4.11
[18:59] Using cautious pH adjust
[18:59] Dispensed 0.000682 mL of Base (0.5 M KOH)
[19:04] Stepping pH = 4.01
[19:04] Dispensed 0.000517 mL of Base (0.5 M KOH)
[19:10] Stepping pH = 4.11
[19:25] Stirrer speed set to 0
[19:35] Datapoint id 12 collected
[19:35] Charge balance equation is out by 12.1%
[19:35] Stirrer speed set to 50
[19:40] pH 4.12 -> 4.32
[19:40] Using charge balance adjust
[19:40] Dispensed 0.001199 mL of Base (0.5 M KOH)
[20:00] Stirrer speed set to 0
[20:11] Datapoint id 13 collected
[20:11] Charge balance equation is out by 71.5%
[20:11] Stirrer speed set to 50
[20:16] pH 4.46 -> 4.66
[20:16] Using cautious pH adjust
[20:16] Dispensed 0.000400 mL of Base (0.5 M KOH)
[20:21] Stepping pH = 4.58
[20:21] Dispensed 0.000188 mL of Base (0.5 M KOH)
[20:26] Stepping pH = 4.68
[20:41] Stirrer speed set to 0
[20:51] Datapoint id 14 collected
[20:51] Charge balance equation is out by 26.5%
[20:51] Stirrer speed set to 50
[20:56] pH 4.73 -> 4.93
[20:56] Using cautious pH adjust
[20:56] Dispensed 0.000259 mL of Base (0.5 M KOH)
[21:02] Stepping pH = 4.86
[21:02] Dispensed 0.000118 mL of Base (0.5 M KOH)
[21:07] Stepping pH = 4.98
[21:22] Stirrer speed set to 0
[21:34] Datapoint id 15 collected
[21:34] Charge balance equation is out by 28.5%
[21:34] Stirrer speed set to 50
[21:39] pH 5.06 -> 5.26

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:39] Using cautious pH adjust
[21:40] Dispensed 0.000141 mL of Base (0.5 M KOH)
[21:45] Stepping pH = 5.13
[21:45] Dispensed 0.000141 mL of Base (0.5 M KOH)
[21:50] Stepping pH = 5.52
[22:05] Stirrer speed set to 0
[22:23] Datapoint id 16 collected
[22:23] Charge balance equation is out by -5.6%
[22:23] Stirrer speed set to 50
[22:29] pH 5.70 -> 5.90
[22:29] Using charge balance adjust
[22:29] Dispensed 0.000094 mL of Base (0.5 M KOH)
[22:49] Stirrer speed set to 0
[23:07] Datapoint id 17 collected
[23:07] Charge balance equation is out by -30.7%
[23:07] Stirrer speed set to 50
[23:12] pH 5.93 -> 6.13
[23:12] Using cautious pH adjust
[23:12] Dispensed 0.000047 mL of Base (0.5 M KOH)
[23:17] Stepping pH = 5.95
[23:17] Dispensed 0.000094 mL of Base (0.5 M KOH)
[23:22] Stepping pH = 7.00
[23:37] Stirrer speed set to 0
[24:37] Datapoint id 18 collected
[24:37] Charge balance equation is out by -81.0%
[24:37] Stirrer speed set to 50
[24:42] pH 8.28 -> 8.48
[24:42] Using cautious pH adjust
[24:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:48] Stepping pH = 8.30
[24:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:53] Stepping pH = 8.31
[24:53] Dispensed 0.000047 mL of Base (0.5 M KOH)
[24:58] Stepping pH = 8.37
[24:58] Dispensed 0.000047 mL of Base (0.5 M KOH)
[25:03] Stepping pH = 8.51
[25:18] Stirrer speed set to 0
[26:03] Datapoint id 19 collected
[26:03] Charge balance equation is out by -1,164.1%
[26:03] Stirrer speed set to 50
[26:08] pH 8.73 -> 8.93
[26:08] Using cautious pH adjust
[26:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:13] Stepping pH = 8.74
[26:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:18] Stepping pH = 8.75
[26:18] Dispensed 0.000094 mL of Base (0.5 M KOH)
[26:23] Stepping pH = 9.13
[26:38] Stirrer speed set to 0
[27:07] Datapoint id 20 collected
[27:07] Charge balance equation is out by -543.2%
[27:07] Titration 2 of 3
[27:07] Adding initial titrants
[27:07] Automatically add 0.08000 mL of Octanol
[27:09] Dispensed 0.080009 mL of Octanol
[27:09] Stirrer speed set to 10
[27:10] Stirrer speed set to 55
[27:10] Iterative adjust 9.27 -> 2.00
[27:10] pH 9.27 -> 2.00

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[27:12] Dispensed 0.054798 mL of Acid (0.5 M HCl)
[27:17] pH 2.02 -> 2.00
[27:17] Dispensed 0.001952 mL of Acid (0.5 M HCl)
[28:07] Stirrer speed set to 0
[28:17] Datapoint id 21 collected
[28:17] Stirrer speed set to 55
[28:22] pH 1.97 -> 2.17
[28:22] Using cautious pH adjust
[28:23] Dispensed 0.009102 mL of Base (0.5 M KOH)
[28:28] Stepping pH = 2.07
[28:28] Dispensed 0.005833 mL of Base (0.5 M KOH)
[28:33] Stepping pH = 2.14
[28:33] Dispensed 0.002516 mL of Base (0.5 M KOH)
[28:39] Stepping pH = 2.17
[28:54] Stirrer speed set to 0
[29:04] Datapoint id 22 collected
[29:04] Charge balance equation is out by 4.1%
[29:04] Stirrer speed set to 55
[29:09] pH 2.17 -> 2.37
[29:09] Using charge balance adjust
[29:10] Dispensed 0.011571 mL of Base (0.5 M KOH)
[29:30] Stirrer speed set to 0
[29:40] Datapoint id 23 collected
[29:40] Charge balance equation is out by 4.1%
[29:40] Stirrer speed set to 55
[29:45] pH 2.39 -> 2.59
[29:45] Using charge balance adjust
[29:46] Dispensed 0.007173 mL of Base (0.5 M KOH)
[30:06] Stirrer speed set to 0
[30:16] Datapoint id 24 collected
[30:16] Charge balance equation is out by -13.1%
[30:16] Stirrer speed set to 55
[30:21] pH 2.57 -> 2.77
[30:21] Using charge balance adjust
[30:21] Dispensed 0.004915 mL of Base (0.5 M KOH)
[30:42] Stirrer speed set to 0
[30:52] Datapoint id 25 collected
[30:52] Charge balance equation is out by -15.1%
[30:52] Stirrer speed set to 55
[30:57] pH 2.75 -> 2.95
[30:57] Using cautious pH adjust
[30:57] Dispensed 0.001764 mL of Base (0.5 M KOH)
[31:02] Stepping pH = 2.81
[31:02] Dispensed 0.002093 mL of Base (0.5 M KOH)
[31:07] Stepping pH = 2.92
[31:07] Dispensed 0.000470 mL of Base (0.5 M KOH)
[31:12] Stepping pH = 2.95
[31:27] Stirrer speed set to 0
[31:37] Datapoint id 26 collected
[31:37] Charge balance equation is out by -22.6%
[31:37] Stirrer speed set to 55
[31:43] pH 2.95 -> 3.15
[31:43] Using cautious pH adjust
[31:43] Dispensed 0.001294 mL of Base (0.5 M KOH)
[31:48] Stepping pH = 3.06
[31:48] Dispensed 0.000753 mL of Base (0.5 M KOH)
[31:53] Stepping pH = 3.12
[31:53] Dispensed 0.000306 mL of Base (0.5 M KOH)
[31:58] Stepping pH = 3.15

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[32:13] Stirrer speed set to 0
[32:23] Datapoint id 27 collected
[32:23] Charge balance equation is out by 9.1%
[32:23] Stirrer speed set to 55
[32:28] pH 3.15 -> 3.35
[32:28] Using charge balance adjust
[32:29] Dispensed 0.002093 mL of Base (0.5 M KOH)
[32:49] Stirrer speed set to 0
[32:59] Datapoint id 28 collected
[32:59] Charge balance equation is out by -11.4%
[32:59] Stirrer speed set to 55
[33:04] pH 3.34 -> 3.54
[33:04] Using charge balance adjust
[33:04] Dispensed 0.001858 mL of Base (0.5 M KOH)
[33:24] Stirrer speed set to 0
[33:34] Datapoint id 29 collected
[33:34] Charge balance equation is out by 3.5%
[33:34] Stirrer speed set to 55
[33:39] pH 3.55 -> 3.75
[33:39] Using charge balance adjust
[33:39] Dispensed 0.001670 mL of Base (0.5 M KOH)
[34:00] Stirrer speed set to 0
[34:10] Datapoint id 30 collected
[34:10] Charge balance equation is out by 67.8%
[34:10] Stirrer speed set to 55
[34:15] pH 3.89 -> 4.09
[34:15] Using cautious pH adjust
[34:15] Dispensed 0.000659 mL of Base (0.5 M KOH)
[34:20] Stepping pH = 4.11
[34:35] Stirrer speed set to 0
[34:46] Datapoint id 31 collected
[34:46] Charge balance equation is out by 50.0%
[34:46] Stirrer speed set to 55
[34:51] pH 4.14 -> 4.34
[34:51] Using cautious pH adjust
[34:51] Dispensed 0.000494 mL of Base (0.5 M KOH)
[34:56] Stepping pH = 4.42
[35:11] Stirrer speed set to 0
[35:22] Datapoint id 32 collected
[35:22] Charge balance equation is out by 50.0%
[35:22] Stirrer speed set to 55
[35:27] pH 4.45 -> 4.65
[35:27] Using cautious pH adjust
[35:27] Dispensed 0.000306 mL of Base (0.5 M KOH)
[35:32] Stepping pH = 4.69
[35:47] Stirrer speed set to 0
[35:59] Datapoint id 33 collected
[35:59] Charge balance equation is out by 50.0%
[35:59] Stirrer speed set to 55
[36:04] pH 4.85 -> 5.05
[36:04] Using cautious pH adjust
[36:04] Dispensed 0.000141 mL of Base (0.5 M KOH)
[36:09] Stepping pH = 4.91
[36:09] Dispensed 0.000165 mL of Base (0.5 M KOH)
[36:14] Stepping pH = 5.80
[36:29] Stirrer speed set to 0
[37:21] Datapoint id 34 collected
[37:21] Charge balance equation is out by -5.2%
[37:21] Stirrer speed set to 55

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[37:27] pH 6.56 -> 6.76
[37:27] Using charge balance adjust
[37:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[37:47] Stirrer speed set to 0
[38:45] Datapoint id 35 collected
[38:45] Charge balance equation is out by -43.3%
[38:45] Stirrer speed set to 55
[38:51] pH 6.84 -> 7.04
[38:51] Using cautious pH adjust
[38:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:56] Stepping pH = 6.89
[38:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:01] Stepping pH = 6.95
[39:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:06] Stepping pH = 7.16
[39:21] Stirrer speed set to 0
[40:21] Datapoint id 36 collected
[40:21] Charge balance equation is out by -119.4%
[40:21] Stirrer speed set to 55
[40:26] pH 7.34 -> 7.54
[40:26] Using cautious pH adjust
[40:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:31] Stepping pH = 7.43
[40:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:36] Stepping pH = 7.48
[40:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:42] Stepping pH = 7.57
[40:57] Stirrer speed set to 0
[41:57] Datapoint id 37 collected
[41:57] Charge balance equation is out by -407.6%
[41:57] Stirrer speed set to 55
[42:02] pH 7.81 -> 8.01
[42:02] Using cautious pH adjust
[42:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:07] Stepping pH = 7.83
[42:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:12] Stepping pH = 7.87
[42:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:17] Stepping pH = 7.91
[42:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:22] Stepping pH = 8.04
[42:37] Stirrer speed set to 0
[43:37] Datapoint id 38 collected
[43:37] Charge balance equation is out by -1,031.4%
[43:37] Stirrer speed set to 55
[43:42] pH 8.38 -> 8.58
[43:42] Using cautious pH adjust
[43:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:48] Stepping pH = 8.40
[43:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:53] Stepping pH = 8.43
[43:53] Dispensed 0.000047 mL of Base (0.5 M KOH)
[43:58] Stepping pH = 8.58
[44:13] Stirrer speed set to 0
[44:58] Datapoint id 39 collected
[44:58] Charge balance equation is out by -519.7%
[44:58] Stirrer speed set to 55
[45:03] pH 8.70 -> 8.90
[45:03] Using cautious pH adjust

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[45:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:08] Stepping pH = 8.70
[45:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[45:13] Stepping pH = 8.71
[45:13] Dispensed 0.000094 mL of Base (0.5 M KOH)
[45:18] Stepping pH = 9.07
[45:33] Stirrer speed set to 0
[45:48] Datapoint id 40 collected
[45:48] Charge balance equation is out by -554.5%
[45:48] Titration 3 of 3
[45:48] Adding initial titrants
[45:48] Automatically add 0.20000 mL of Octanol
[45:53] Dispensed 0.200000 mL of Octanol
[45:53] Stirrer speed set to 10
[45:54] Stirrer speed set to 60
[45:54] Iterative adjust 9.28 -> 2.00
[45:54] pH 9.28 -> 2.00
[45:55] Dispensed 0.057761 mL of Acid (0.5 M HCl)
[46:00] pH 2.01 -> 2.00
[46:01] Dispensed 0.001294 mL of Acid (0.5 M HCl)
[46:51] Stirrer speed set to 0
[47:01] Datapoint id 41 collected
[47:01] Stirrer speed set to 60
[47:06] pH 1.97 -> 2.17
[47:06] Using cautious pH adjust
[47:06] Dispensed 0.009901 mL of Base (0.5 M KOH)
[47:11] Stepping pH = 2.05
[47:12] Dispensed 0.007926 mL of Base (0.5 M KOH)
[47:17] Stepping pH = 2.13
[47:17] Dispensed 0.003057 mL of Base (0.5 M KOH)
[47:22] Stepping pH = 2.17
[47:37] Stirrer speed set to 0
[47:48] Datapoint id 42 collected
[47:48] Charge balance equation is out by -5.4%
[47:48] Stirrer speed set to 60
[47:53] pH 2.17 -> 2.37
[47:53] Using charge balance adjust
[47:53] Dispensed 0.012488 mL of Base (0.5 M KOH)
[48:14] Stirrer speed set to 0
[48:24] Datapoint id 43 collected
[48:24] Charge balance equation is out by -4.2%
[48:24] Stirrer speed set to 60
[48:29] pH 2.37 -> 2.57
[48:29] Using charge balance adjust
[48:29] Dispensed 0.008184 mL of Base (0.5 M KOH)
[48:49] Stirrer speed set to 0
[49:00] Datapoint id 44 collected
[49:00] Charge balance equation is out by -4.0%
[49:00] Stirrer speed set to 60
[49:05] pH 2.57 -> 2.77
[49:05] Using charge balance adjust
[49:05] Dispensed 0.005503 mL of Base (0.5 M KOH)
[49:25] Stirrer speed set to 0
[49:35] Datapoint id 45 collected
[49:35] Charge balance equation is out by -14.9%
[49:35] Stirrer speed set to 60
[49:40] pH 2.74 -> 2.94
[49:40] Using charge balance adjust
[49:41] Dispensed 0.004022 mL of Base (0.5 M KOH)

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[50:01] Stirrer speed set to 0
[50:11] Datapoint id 46 collected
[50:11] Charge balance equation is out by -5.7%
[50:11] Stirrer speed set to 60
[50:16] pH 2.94 -> 3.14
[50:16] Using charge balance adjust
[50:16] Dispensed 0.003057 mL of Base (0.5 M KOH)
[50:36] Stirrer speed set to 0
[50:46] Datapoint id 47 collected
[50:46] Charge balance equation is out by 0.9%
[50:46] Stirrer speed set to 60
[50:52] pH 3.14 -> 3.34
[50:52] Using charge balance adjust
[50:52] Dispensed 0.002446 mL of Base (0.5 M KOH)
[51:12] Stirrer speed set to 0
[51:22] Datapoint id 48 collected
[51:22] Charge balance equation is out by 52.1%
[51:22] Stirrer speed set to 60
[51:27] pH 3.45 -> 3.65
[51:27] Using cautious pH adjust
[51:28] Dispensed 0.000917 mL of Base (0.5 M KOH)
[51:33] Stepping pH = 3.65
[51:48] Stirrer speed set to 0
[51:58] Datapoint id 49 collected
[51:58] Charge balance equation is out by 50.0%
[51:58] Stirrer speed set to 60
[52:03] pH 3.65 -> 3.85
[52:03] Using cautious pH adjust
[52:03] Dispensed 0.000729 mL of Base (0.5 M KOH)
[52:08] Stepping pH = 3.89
[52:23] Stirrer speed set to 0
[52:33] Datapoint id 50 collected
[52:33] Charge balance equation is out by 50.0%
[52:33] Stirrer speed set to 60
[52:38] pH 3.90 -> 4.10
[52:38] Using cautious pH adjust
[52:39] Dispensed 0.000517 mL of Base (0.5 M KOH)
[52:44] Stepping pH = 4.06
[52:44] Dispensed 0.000094 mL of Base (0.5 M KOH)
[52:49] Stepping pH = 4.08
[52:49] Dispensed 0.000071 mL of Base (0.5 M KOH)
[52:54] Stepping pH = 4.12
[53:09] Stirrer speed set to 0
[53:19] Datapoint id 51 collected
[53:19] Charge balance equation is out by 33.8%
[53:19] Stirrer speed set to 60
[53:24] pH 4.14 -> 4.34
[53:24] Using cautious pH adjust
[53:24] Dispensed 0.000353 mL of Base (0.5 M KOH)
[53:29] Stepping pH = 4.47
[53:44] Stirrer speed set to 0
[53:54] Datapoint id 52 collected
[53:54] Charge balance equation is out by 50.0%
[53:54] Stirrer speed set to 60
[54:00] pH 4.52 -> 4.72
[54:00] Using cautious pH adjust
[54:00] Dispensed 0.000165 mL of Base (0.5 M KOH)
[54:05] Stepping pH = 4.67
[54:05] Dispensed 0.000047 mL of Base (0.5 M KOH)

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[54:10] Stepping pH = 4.69
[54:10] Dispensed 0.000047 mL of Base (0.5 M KOH)
[54:15] Stepping pH = 4.78
[54:30] Stirrer speed set to 0
[54:43] Datapoint id 53 collected
[54:43] Charge balance equation is out by 22.1%
[54:43] Stirrer speed set to 60
[54:48] pH 4.89 -> 5.09
[54:48] Using cautious pH adjust
[54:48] Dispensed 0.000071 mL of Base (0.5 M KOH)
[54:53] Stepping pH = 4.94
[54:53] Dispensed 0.000118 mL of Base (0.5 M KOH)
[54:58] Stepping pH = 6.12
[55:13] Stirrer speed set to 0
[55:51] Datapoint id 54 collected
[55:51] Charge balance equation is out by -21.1%
[55:51] Stirrer speed set to 60
[55:56] pH 6.13 -> 6.33
[55:56] Using cautious pH adjust
[55:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:01] Stepping pH = 6.16
[56:01] Dispensed 0.000071 mL of Base (0.5 M KOH)
[56:06] Stepping pH = 6.51
[56:21] Stirrer speed set to 0
[57:21] Datapoint id 55 collected
[57:21] Charge balance equation is out by -82.3%
[57:21] Stirrer speed set to 60
[57:26] pH 6.85 -> 7.05
[57:26] Using cautious pH adjust
[57:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:31] Stepping pH = 6.94
[57:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:37] Stepping pH = 7.01
[57:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:42] Stepping pH = 7.10
[57:57] Stirrer speed set to 0
[58:57] Datapoint id 56 collected
[58:57] Charge balance equation is out by -92.6%
[58:57] Stirrer speed set to 60
[59:02] pH 7.25 -> 7.45
[59:02] Using cautious pH adjust
[59:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:07] Stepping pH = 7.33
[59:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:12] Stepping pH = 7.49
[59:27] Stirrer speed set to 0
[1:00:27] Datapoint id 57 collected
[1:00:27] Charge balance equation is out by -136.9%
[1:00:27] Stirrer speed set to 60
[1:00:32] pH 7.57 -> 7.77
[1:00:32] Using cautious pH adjust
[1:00:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:38] Stepping pH = 7.65
[1:00:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:43] Stepping pH = 7.74
[1:00:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:48] Stepping pH = 7.91
[1:01:03] Stirrer speed set to 0
[1:02:03] Datapoint id 58 collected

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-27016**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-27016_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **2/27/2018 10:54:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:02:03] Charge balance equation is out by -478.6%
[1:02:03] Stirrer speed set to 60
[1:02:08] pH 8.11 -> 8.31
[1:02:08] Using cautious pH adjust
[1:02:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:13] Stepping pH = 8.12
[1:02:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:18] Stepping pH = 8.20
[1:02:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:24] Stepping pH = 8.30
[1:02:39] Stirrer speed set to 0
[1:03:30] Datapoint id 59 collected
[1:03:30] Charge balance equation is out by -552.5%
[1:03:30] Stirrer speed set to 60
[1:03:35] pH 8.41 -> 8.61
[1:03:35] Using cautious pH adjust
[1:03:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:40] Stepping pH = 8.43
[1:03:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:45] Stepping pH = 8.46
[1:03:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:03:50] Stepping pH = 8.58
[1:03:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:56] Stepping pH = 8.71
[1:04:11] Stirrer speed set to 0
[1:04:35] Datapoint id 60 collected
[1:04:35] Charge balance equation is out by -623.7%
[1:04:35] Stirrer speed set to 60
[1:04:40] pH 8.77 -> 8.97
[1:04:40] Using cautious pH adjust
[1:04:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:45] Stepping pH = 8.78
[1:04:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:04:50] Stepping pH = 8.84
[1:04:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:04:55] Stepping pH = 8.97
[1:05:11] Stirrer speed set to 0
[1:05:37] Datapoint id 61 collected
[1:05:37] Charge balance equation is out by -302.6%
[1:05:37] Stirrer speed set to 60
[1:05:42] pH 9.03 -> 9.05
[1:05:42] Using cautious pH adjust
[1:05:57] Stirrer speed set to 0
[1:06:16] Datapoint id 62 collected
[1:06:16] Charge balance equation is out by 100.0%
[1:06:16] Argon flow rate set to 0
[1:06:20] Titrator arm moved over Titration position